

## ROCK EVALUATION

### Introduction

Rock Evaluation analyses were used to evaluate type and maturity of organic matter, calculate petroleum potential, and detect oil shows. These measurements are usually done by exploration companies looking for oil and gas. The Rock Evaluation (RE) data were generated using the Delsi Nermag Rock-Eval II Plus TOC instrument for whole rock or sediment pyrolysis.

Oil exploration was not the reason that rock evaluation analyses were done by the Ocean Drilling Program (ODP). There was a significant amount of planning and research done to avoid drilling in areas that had potential for oil or gas. These data were used on the ship as an interpretive tool for monitoring hydrocarbon safety levels, in addition to providing information about the organic matter in the sediments. Because of the length of time necessary to complete the analysis of a sample, RE results were not normally used as a part of the real-time hydrocarbon monitoring program.

### Data Acquisition

Rock Evaluation data (RE or rock eval) have been collected since ODP Leg 101 on the Delsi-Nermag Rock Eval II Plus TOC instrument. Samples analyzed for rock evaluation were usually subsamples of the freeze-dried and crushed material collected for carbon analyses. The Rock Evaluation method consisted of programmed temperature heating to quantitatively determine any free hydrocarbons contained in the sample and the hydrocarbon- and oxygen-containing compounds that are volatilized during heating.

Five basic parameters --  $S_1$ ,  $S_2$ ,  $S_3$ , temperature max ( $T_{max}$ ) and total organic carbon (TOC) -- were measured.

- $S_1$  – amount of free hydrocarbons (gas and oil). If  $S_1 > 1$  mg/g, it may be indicative of an oil show.  $S_1$  can be contaminated by the drilling fluids and mud.
- $S_2$  – the amount of hydrocarbons generated through thermal cracking of nonvolatile organic matter.  $S_2$  is an indication of the quantity of hydrocarbons the sediments could potentially produce should burial and maturation continue.
- $S_3$  – the amount of  $CO_2$  produced during pyrolysis of kerogen.  $S_3$  is an indication of the amount of oxygen in the kerogen.
- $T_{max}$  – the temperature at which the maximum release of hydrocarbons from cracking of kerogen occurs during pyrolysis.  $T_{max}$  is an indication of the stage of maturation of the organic matter.
- TOC – total organic carbon (weight percent) can be determined by oxidizing the organic matter remaining in the sample after pyrolysis. The TOC is determined by adding this residual organic carbon to the pyrolyzed organic carbon.

From those measurements, four additional parameters can be calculated that describe the type and maturity of the organic matter:

- Productivity Index (PI) –  $[S_1 / (S_1 + S_2)]$  characterizes the evolution level of the organic matter. In an ideal situation with increasing burial depth,  $S_1$  should increase and  $S_2$  should decrease resulting with PI increasing with depth and maturation.
- Petroleum Potential or Pyrolyzed Carbon (PC) –  $[0.083 \times (S_1 + S_2)]$  corresponds to carbon content, the maximum quantity of hydrocarbons capable of being produced from the source rock, given sufficient depth and time.
- Hydrogen Index (HI) –  $[(100 \times S_2) / \text{TOC}]$  is a parameter used to characterize the origin of the organic material. Marine organisms and algae have higher hydrogen-to-carbon ratios than land plants. HI typically ranges from ~100 to 600 in geological samples.
- Oxygen Index (OI) –  $[(100 \times S_3) / \text{TOC}]$  is a parameter that indirectly correlates the ratio of oxygen to carbon. OI values range from ~0 to 150.

Additional information about rock evaluation measurements can be found in Technical Note 30: Introduction to Shipboard Organic Geochemistry on the *JOIDES Resolution*.

## Archive

### Pre-Janus Archive

Early in the ODP, Rock Eval data were collected on logsheets which were sent back to ODP/TAMU at the end of each cruise. The data were entered into an S1032 database and the logsheets were microfilmed for archival storage. Data entry routines were implemented so that data entry could be done on the ship. Rock Eval data were stored in the S1032 database until the Janus database became operational on Leg 171.

### Migration of Rock Evaluation data to Janus

The data model for Rock Eval data can be found in Appendix I. Included are the relational diagram and the list of the tables that contain data pertinent to Rock Eval, the column names and the definition of each column attribute. ODP Information Services Database Group was responsible for the migration of pre-Leg 171 data to Janus. When the Janus data model was implemented, tables to store RE data were created. After Janus became operational, it was determined that it was more practical to store the data in the Carbonate tables, especially since many of the rock eval analyses were done on splits of the carbonate samples.

Organic carbon (ORG\_C) determined by coulometer as part of the carbonate analyses was often used instead of the TOC measurement from the RE instrument to calculate the parameters HI and OI. One problem that recurred periodically throughout the

migration was determining whether the organic carbon value was ORG\_C (coulometer) or TOC (RE). The tables in the Initial Report volumes often did not discriminate between the ORG\_C and TOC.

### Janus Rock Evaluation Data Format

Rock eval analyses can be retrieved from Janus Web using a predefined query. The Rock Eval query webpage allows the user to extract data using the following variables to restrict the amount of data retrieved: leg, site, hole, core, section, depth, or latitude and longitude ranges. In addition, this query includes the organic carbon values obtained from the carbonate analysis. Often, this value was used in place of TOC to calculate the parameters, HI and OI.

Table 1 lists the data fields retrieved from the Janus database for the Rock Eval predefined query. The first column contains the data item; the second column indicates the Janus table or tables in which the data were stored; the third column is the Janus column name or the calculations used to produce the value. Appendix II contains additional information about the fields retrieved using the Janus Web Rock Eval query, and the data format for the archived ASCII files.

Table 1. Rock Eval Query

Item Name	Janus Table	Janus Column Name and Calculation
Leg	SECTION	Leg
Site	SECTION	Site
Hole	SECTION	Hole
Core	SECTION	Core
Coretype	SECTION	Core_type
Section	SECTION	Section_number
Top Interval	SAMPLE	Top_Interval x 100
Bottom Interval	SAMPLE	Bottom_Interval x 100
Depth (mbsf)	DEPTH_MAP, SAMPLE	DEPTH_MAP.Map_interval_top + SAMPLE.Top_interval
Organic Carbon (wt %)	CHEM_CARB_ANALYSIS	Analysis_code - ORG_C::Analysis_result
Total Organic Carbon (wt %)	CHEM_CARB_ANALYSIS	Analysis_code - TOC::Analysis_result
Free Hydrocarbons (S1) [mg HC/g]	CHEM_CARB_ANALYSIS	Analysis_code - S1::Analysis_result
Hydrocarbons (S2) [mg HC/g]	CHEM_CARB_ANALYSIS	Analysis_code - S2::Analysis_result
Carbon Dioxide (S3) [mg CO2/g]	CHEM_CARB_ANALYSIS	Analysis_code - S3::Analysis_result
Max Temperature (TMX) [Deg C]	CHEM_CARB_ANALYSIS	Analysis_code - TMX::Analysis_result
Productivity Index (PI) [ratio]	CHEM_CARB_ANALYSIS	Analysis_code - PI::Analysis_result
Petroleum Potential (PC) [mg HC/g]	CHEM_CARB_ANALYSIS	Analysis_code - PC::Analysis_result
Oxygen Index (OI) [ratio]	CHEM_CARB_ANALYSIS	Analysis_code - OI::Analysis_result
Hydrogen Index (HI) [ratio]	CHEM_CARB_ANALYSIS	Analysis_code - HI::Analysis_result

### Data Quality

The Rock Eval data in Janus represents an extensive collection of organic carbon analyses in sediments from ocean basins throughout the earth. Over 9,300 samples were analyzed to characterize organic carbon. A common error found during the

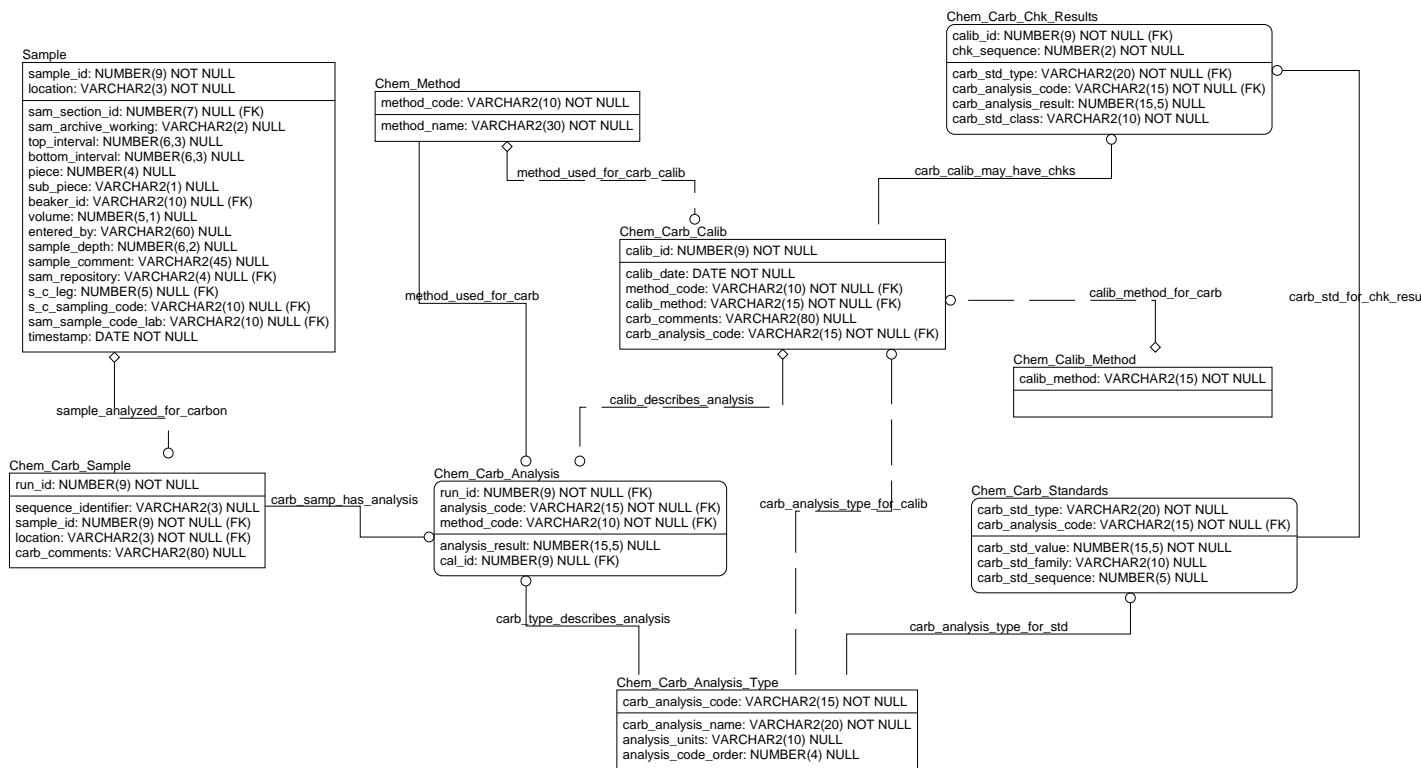
migration was that samples were missing from the database. In those instances, a sample was entered into the database so that the data could be migrated. Another common error falls in the general category of operator error. Analytical results were written on logsheets. These data were then typed into S1032. Data entry programs were implemented to add the data to S1032, but it still required manual entry. Data acquisition programs were later implemented to collect rock eval data, but the operator manually entered the sample information. Mistakes in logging samples, logging data, typing data into the database, etc. occasionally happened, and were not always identified. Often, the scientific party found errors and corrected them for the data included in the Initial Report volume, but data sent back to ODP/TAMU did not get corrected.

Verification of the entire rock eval data set was not completed due to time constraints. One result of this is that the ORG\_C data does not always get retrieved, even though it exists in Janus. If ORG\_C data are missing from the Rock Eval query, those data should be available through the Carbonate query. Most data collected after the Janus database was operational on Leg 171 were verified as part of the Janus data management and verification procedures (see Metadata Introduction). Some verification was done on the pre-Leg 171 data; however, if there is a discrepancy between the database and data in the Initial Report volumes, the published data should be considered more reliable.

Janus does not contain any calibration information for rock eval. Procedures for storing calibration information were not implemented during the ODP.

## References

- Emeis, K., and Kvenvolden, K.A., 1986. Shipboard Organic Geochemistry on *JOIDES Resolution*, ODP Tech. Note No. 7.
- Kvenvolden, K.A., and McDonald, T.J., 1986. Organic Geochemistry on the *JOIDES Resolution*--An Assay, ODP Tech. Note No. 6.
- Pimmel, A., and Claypool, G., 2001, Introduction to Shipboard Organic Geochemistry on the *JOIDES Resolution*. ODP Tech. Note 30.



## APPENDIX I: Janus Data Model – Rock Evaluation (stored in Carbonate tables)

<b>Rock Evaluation – RE</b>		
<b>Table Name</b>	<b>Column Name</b>	<b>Column Comment</b>
<b>Chem_Carb_Sample</b>	run_id	Unique Oracle-generated sequence identifier that will allow duplicate analyses of a sample to be entered into database.
	sequence_identifier	Number indicating order in which analyses were run when duplicate analyses are stored.
	sample_id	Oracle-generated sequence number that with /location uniquely identifies a sample.
	location	Code that indicates which Janus application assigned the sample_id. Used with sample_id to uniquely identify a sample.
	carb_comments	Comment concerning a rock evaluation analysis.
<b>Chem_Carb_Analysis</b>	run_id	Unique Oracle-generated sequence identifier that will allow duplicate analyses of a sample to be entered into database.
	analysis_code	Code describing the type of analysis for which a sample was analyzed.
	method_code	A code for the method or instrument used to analyze a sample.
	analysis_result	Numerical result of the analysis of a sample.
	cal_id	Oracle-generated sequence number for a calibration run.
<b>Chem_Carb_Analysis_Type</b>	carb_analysis_code	Code describing the type of analysis for which a sample can be analyzed.
	carb_analysis_name	Full name or description of analysis type.
	analysis_units	The reported measurement units of the analysis result.
	analysis_code_order	Number defining the order that analysis codes and results will appear on a spreadsheet or report.
<b>Chem_Method</b>	method_code	A code for the method or instrument used for analyzing a sample.
	method_name	The name of the method or instrument used for analyzing a sample.
<b>Chem_Carb_Calib</b>	calib_id	Oracle-generated sequence number for a calibration run.
	calib_date	The date and time of a calibration run.
	method_code	A code for the method or instrument used for analyzing a sample.
	calib_method	Method used for calibrating the analytical instrument.
	carb_comments	A comment concerning a calibration.
	carb_analysis_code	Code describing the type of analysis for which a sample can be analyzed.
<b>Chem_Calib_Method</b>	calib_method	Method used for calibrating the analytical instrument.
<b>Chem_Carb_Chk_Results</b>	calib_id	Oracle-generated sequence number for a calibration run.
	chk_sequence	Number indicating order of measurements.
	carb_std_type	The name of the standard used.
	carb_analysis_code	Code describing the type of analysis for which a sample can be analyzed.
	carb_analysis_result	The result of the analysis of a sample or standard.
	carb_std_class	Code describing type of check analysis as a standard, blank, or unknown check
<b>Chem_Carb_Standards</b>	carb_std_type	The name of the standard used.
	carb_analysis_code	Code describing the type of analysis for which a sample can be analyzed.
	carb_std_value	The value of a standard for a particular analysis code.
	carb_std_family	Name for a group of standards.
	carb_std_sequence	

## Rock Evaluation – RE

Table Name	Column Name	Column Comment
Section	section_id	Unique Oracle-generated sequence number to identify each section. This is done because of the physical subsection / zero section problems. In adding new sections, deleting sections or changing sections - don't want to have to renumber.
	leg	Number identifying the cruise for which data were entered into the database.
	site	Number identifying the site from which the core was retrieved. A site is the position of a beacon around which holes are drilled.
	hole	Letter identifying the hole at a site from which a core was retrieved or data were collected.
	core	Sequential numbers identifying the cores retrieved from a particular hole. Cores are generally 9.5 meters in length, and are numbered serially from the top of the hole downward.
	core_type	A letter code identifying the drill bit/coring method used to retrieve the core.
	section_number	Cores are cut into 1.5 m sections. Sections are numbered serially, with Section 1 at the top of the core.
	section_type	Used to differentiate sections of core (S) from core catchers (C). Previously core catchers were stored as section CC, but in Janus core catchers are given the next sequential number from the last section recovered.
	curated_length	The length of the section core material, in meters. This may be different than the liner length for the same section. Hard rock cores will often have spacers added to prevent rock pieces from damaging each other.
	liner_length	The original length of core material in the section, in meters. Sum of liner lengths of all the sections of a core equals core recovery.
	core_catcher_stored_in	Sometimes the core catcher is stored in a D tube with a section. core_catcher_stored_in contains the section number of the D tube that holds the core catcher.
	section_comments	Comments about this section

Sample	sample_id	Oracle-generated sequence number that with location uniquely identifies a sample.
	location	Code that indicates which Janus application assigned the sample_id. Values are SHI (ship), GCR (Gulf Coast Repository), ECR (East Coast Repository, WCR (West Coast Repository) and BCR (Bremen Core Repository). Used with sample_id to uniquely identify a sample.
	s_c_leg	Number identifying the cruise for which data were entered into the database. Foreign key used with s_c_sampling_code to link samples with a scientist's sample request.
	s_c_sampling_code	Code used to identify samples taken for a sample request. Used with s_c_leg.
	sam_archive_working	Part of section where sample was taken. Valid values: WR – whole round, A – archive half, W – working half.
	top_interval	Distance in meters from the top of the section to the top of the sample.
	bottom_interval	Distance in meters from the top of the section to the bottom of the sample.
	piece	Additional identifier for hard rock samples. Each individual piece of rock within a section is numbered consecutively starting at the top of the section.
	sub_piece	Additional identifier for hard rock samples. When a piece is broken, the individual fragments are given consecutive letter designations. Note that subpiece assignments must be made in conjunction with piece numbers.
	beaker_id	The number on the moisture density beaker. Used for samples analyzed for moisture and density.
	volume	Volume of sample.
	entered_by	Indicates who entered the sample into the database.
	sample_depth	Depth of the sample.
	sample_comment	Comment about the sample.
	sam_repository	Repository where sample was taken. Valid values SHIP (ship), GCR (Gulf Coast Repository), ECR (East Coast Repository), WCR (West Coast Repository) and BCR (Bremen Core Repository).
	sam_sample_code_lab	Code to indicate the shipboard lab that will perform the initial analysis.
	sam_section_id	Unique Oracle-generated sequence number to identify each section. This is a foreign key that links a sample to leg, site, hole, core, and section.
	timestamp	Date and time when sample was entered into database. Samples taken before November 25, 1998 and migrated samples have the timestamp 11/25/1998 12:26 PM.

## Appendix II: Description of data items from Rock Eval query

Column Name	Column Description and Calculations	Format
Leg	Number identifying the cruise. The ODP started numbering the scientific cruises of the <i>JR</i> at Leg 101. A leg was nominally two months duration. During the 18+ years of the ODP, there were 110 cruises on the <i>JR</i> .	Integer 3
Site	Number identifying the site. A site is the location where one or more holes were drilled while the ship was positioned over a single acoustic beacon. The <i>JR</i> visited 656 unique sites during the course of the ODP. Some sites were visited multiple times, including some sites originally visited during the Deep Sea Drilling Program for a total of 673 site visits.	Integer 4
Hole	Letter identifying the hole. Multiple holes could be drilled at a single site by pulling the drill pipe above the seafloor, moving the ship some distance away and drilling another hole. The first hole was designated 'A' and additional holes proceeded alphabetically at a given site. Location information for the cruise was determined by Hole latitude and longitude. During ODP, there were 1818 holes drilled or deepened.	Text 1
Core	Cores are numbered serially from the top of the hole downward. Cored intervals are up to 9.7 m long, the maximum length of the core barrel. Recovered material was placed at the top of the cored interval, even when recovery was less than 100%. More than 220 km of core were recovered by the ODP.	Integer 3
Coretype	All cores are tagged by a letter code that identifies the coring method used.	Text 1
Section	Cores are cut into 1.5 m sections in order to make them easier to handle. Sections are numbered serially, with Section 1 at the top of the core. Rock Evaluation measurements were made on samples taken from the sections. Samples taken from the Core Catcher sections are identified as "CC".	Integer 2 or Text 2
Top Interval	The top interval of a measurement in centimeters measured from the top of a section.	Decimal F4.1
Bottom Interval	The location of the bottom of a sample within a section, in centimeter.s	Decimal F4.1
Depth (mbsf)	Distance in meters from the seafloor to the sample location.	Decimal F7.3
Organic Carbon (wt %)	The weight percent of organic carbon in a sample, from the carbonate analysis of the sample. This value can be measured directly or calculated by subtracting the Inorganic_Carbon_Percent from the Total_Carbon_Percent.	Decimal F15.5
Total Organic Carbon (wt %)	Total Organic Carbon in weight percent. This value is obtained from the RE-TOC apparatus.	Decimal F15.5
Free Hydrocarbons (S1) [mg HC/g]	This peak represents the quantity (in mg hydrocarbon/g rock) of free hydrocarbons (oil and gas) present, which are volatilized below 300 °C.	Decimal F15.5
Hydrocarbons (S2) [mg HC/g]	The amount of hydrocarbon-type compounds (in mg hydrocarbon/g rock) produced by the cracking of kerogen as the temperature increases to 600 degrees C. This also indicates the quantity of hydrocarbons which could be produced should burial and maturation continue.	Decimal F15.5
Carbon Dioxide (S3) [mg CO <sub>2</sub> /g]	This peak shows the quantity of CO <sub>2</sub> (measured in mg CO <sub>2</sub> /g rock) produced from pyrolysis of the organic matter in the rock up to 390 degrees C.	Decimal F15.5

<b>Column Name</b>	<b>Column Description and Calculations</b>	<b>Format</b>
Temperature MAX [Deg C]	The temperature (in °C) at which maximum release of hydrocarbons from cracking of kerogen during pyrolysis occurred (measured at peak of S2).	Decimal F15.5
Productivity Index (PI) [ratio]	S1/(S1 + S2). PI characterizes the evolution level of the organic matter. PI typically increases with depth and can be used to pinpoint zones of unusually high or low amounts of hydrocarbons.	Decimal F15.5
Pyrolyzed Carbon (PC) [mg HC/g]	Petroleum Potential or Pyrolyzed Carbon = k x (S1 + S2), where k = 0.083 mg carbon/g rock. PC corresponds to the maximum quantity of hydrocarbons capable of being produced from the source rock or sediment given sufficient burial depth and time.	Decimal F15.5
Oxygen Index (OI) [ratio]	OI = (100 x S3)/TOC. OI indirectly determines the ratio of oxygen to carbon. It is also used to evaluate the type of organic matter present.	Decimal F15.5
Hydrogen Index (HI) [ratio]	Hydrogen Index = (100 x S2)/TOC. HI indirectly determines the ratio of hydrogen to carbon. It is a parameter used to evaluate the type of organic matter present.	Decimal F15.5